

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.84            | 0.55 | 0.85           | 0.53 | 0.83       | 0.64 |

Model Results

Predicted value: 6.47e-01

Global applicability domain: Inside

Local applicability domain index: 3.52e-01

Confidence level: 7.17e-01

Nearest Neighbors from the Training Set

|   |  |   |
|---|--|---|
| <div>Image not found</div> <div>Dichlorvos</div> <div>Measured: 5.01e-01</div> <div>Predicted: 6.47e-01</div>               | <div>Image not found</div> <div>Tris(2-chloroethyl) phosphate</div> <div>Measured: 1.29</div> <div>Predicted: 1.66</div> | <div>Image not found</div> <div>Triethyl phosphate</div> <div>Measured: 1.29</div> <div>Predicted: 1.38</div> |
| <div>Image not found</div> <div>Tris(2-chloroisopropyl)phosphate</div> <div>Measured: 7.94</div> <div>Predicted: 6.64</div> | <div>Image not found</div> <div>Trimethyl phosphate</div> <div>Measured: 1.41</div> <div>Predicted: 1.50</div>           |   |